BIOMATH
Department of Applied Mathematics,
Biometrics and Process Control

Optimal Experimental Design in River Water Quality Modelling

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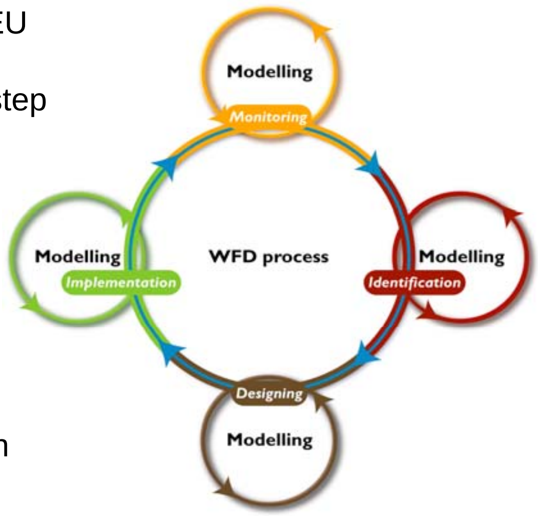
Overview

- Introduction
- Aim
- ESWAT
- Dender case
- Methodology
- Results
- Conclusion

Introduction

Monitoring

- For implementation of the EU Water Framework Directive monitoring is an important step for identification/evaluation.
- Models can play a role in every step.
- Hence, also the monitoring needed to build models for evaluation of future pollution abatement scenarios



Introduction

Monitoring problems

- Costly measurements: e.g. BOD, suspended solids, micro-pollutants
- Measurements with wrong frequency, in non-sensitive periods, on wrong places
- Lot of effort needed to maintain large databases
- Intensive measurement campaigns

Objective

- Calibration of water quality models
  - identifiability of the model parameters
  - reliability of the model (uncertainty analysis)

=> depends on good measurements

Find an optimal set of sampling data for the calibration of a water quality model

ESWAT

Integrated modelling tool

SWAT 98

- Catchment hydrology
- Agricultural pollution
- Constant point sources

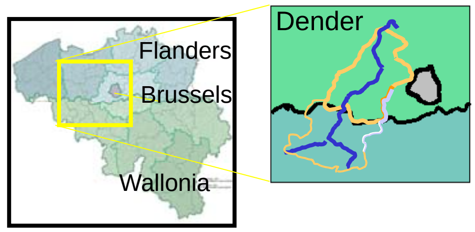
ESWAT (van Griensven)

- Hourly time step (land and river hydrology)
- River water quality processes
- Dynamic point sources
- Urban drainage system

Dender case

Dender basin

- 1400 km² catchment
- 50 km long river stretch
- Flemish part modelled
  - heavily polluted
  - sluices for navigation
  - 85% agriculture, 15% urban
  - 300,000 inhabitants (400/km²)

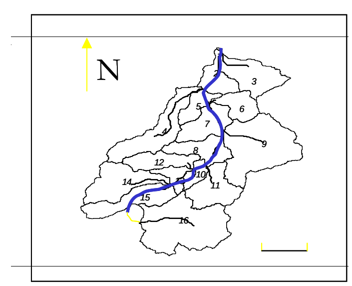


Dender case

Dender basin model

MODEL: 700 km²

- 15 subbasins / 8 tributaries
- 80 HRU's (=combination land use and soil type)
- 10 point source locations
- 8 sluices

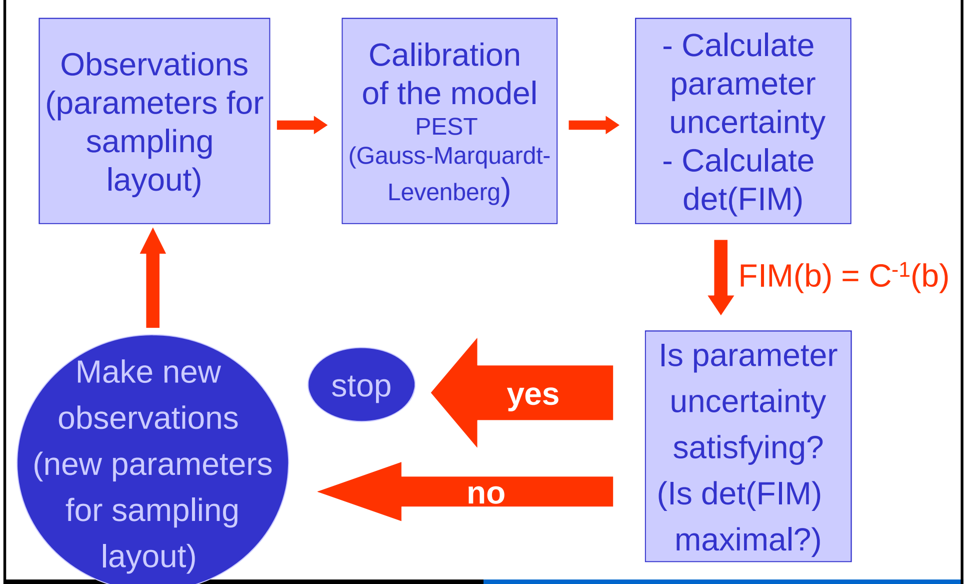


Methodology

Optimal Experimental Design

- Start with a calibrated model,
  but with large uncertainty bounds caused by
  a lack of good measurements to do a good calibration
- Perform virtual experiments (generate time series)
  with the model for water quality variables of interest
- See where, when, how many measurements/samples
  are practically and economically feasible
  and define the parameters of the sampling layout

Methodology

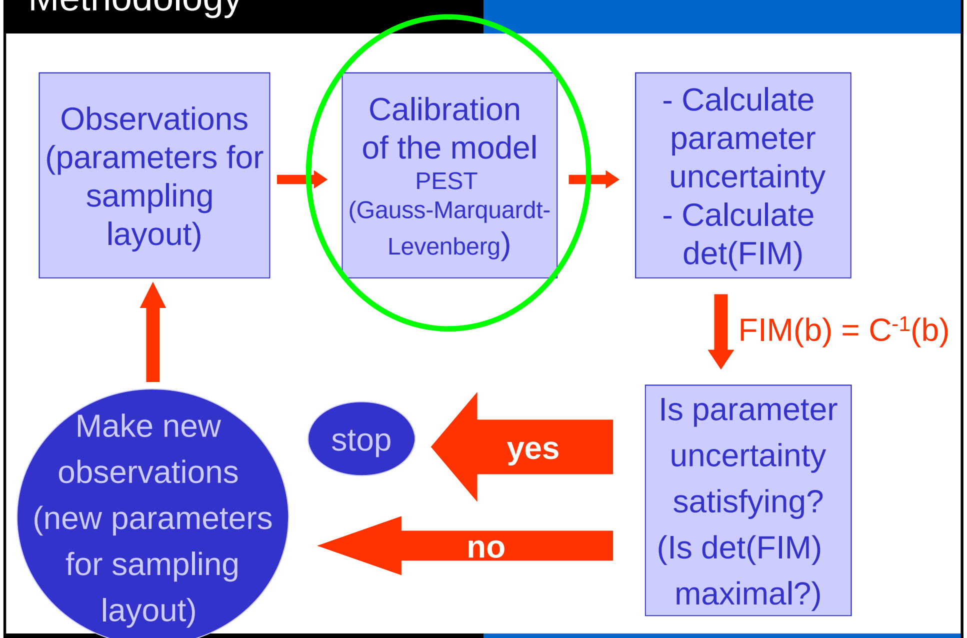


Methodology

Virtual Observations

- No historic time series
  of high frequency water quality data available
- => Virtual observation series generated by ESWAT
  + pseudo-random noise terms
- Noise terms: consistent with the accuracy of the measurement devices
- Parameters for sampling design:
  variable, measurement location, frequency, timing
  e.g. every 12 hours, at the mouth + 5km more upstream,
  from 01/04 till 31/08

Methodology



Methodology

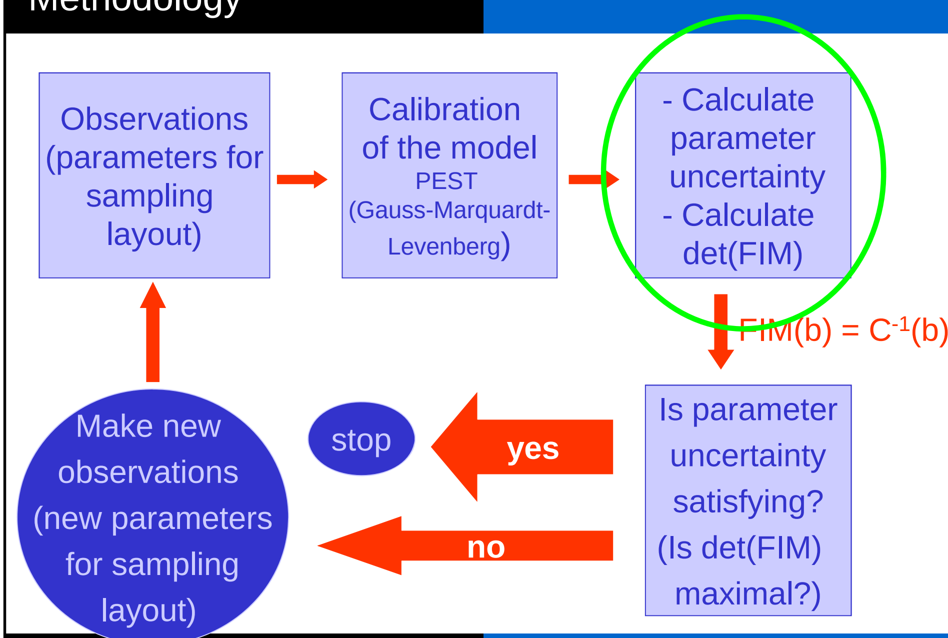
Virtual Calibration

- Start calibration at a point 'close' to the former calibration (to avoid local minima/converge quickly)

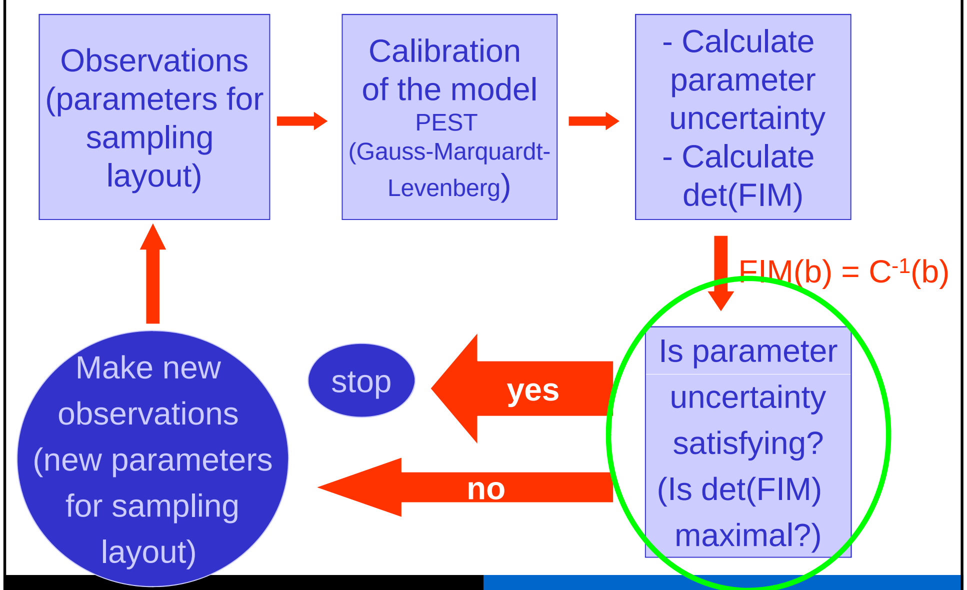
During the calibration the covariance matrix and the uncertainty bounds on the parameters are calculated

- PEST: uses Gauss-Marquardt-Levenberg

Methodology



Methodology



Methodology

D-optimal design method

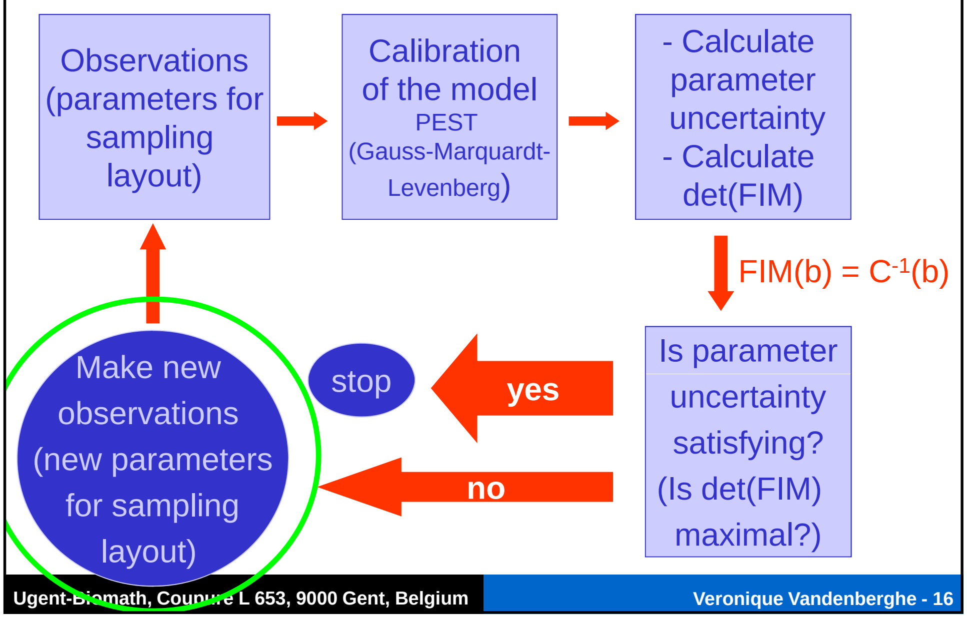
- New measurement layout => with D-optimal design method (= maximisation of Det(FIM))

$$C(b) = \partial^2 (J^t Q J)$$

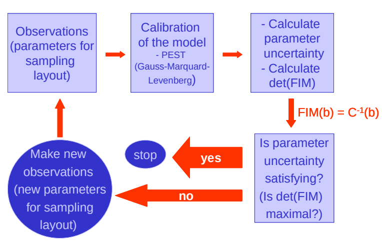
$$Fisher\ Information\ Matrix = C^{-1}(b)$$

- Maximisation of Det(FIM) with shuffled complex technique (SCE-UA method) by changing parameters of sampling layout (frequency, location, timing,…)

Methodology



Methodology



- **When 'STOP' = make actual measurements following the obtained sampling parameters**
- **Then start the procedure all over again =>iterative method**
- **The sampling procedure can change year after year, following natural trends, e.g. climate change or human interventions, such as a dam, a new discharge point, ...**

Results

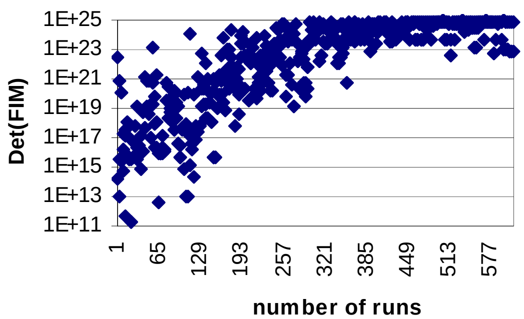
OED for Dender basin

Five parameters of the sample layout variable:

- **Frequency: every hour - every two days**
- **Timing: summer, winter, mixed summer-winter**
- **Total number of samples (365*24)**
- **Variables: only DO or combined DO-NO_3, DO-NO_3-BOD or DO-NO_3-BOD-NH_4**
- **Sample location: 4 possible combinations of 3 possible locations: upstream, halfway, downstream**

Results

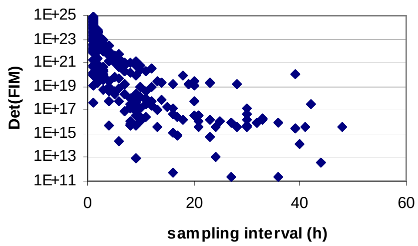
OED for Dender basin

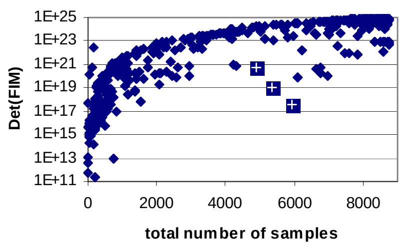


- 635 iterations needed

Results

OED for Dender basin





- **Best : hourly time base, nearly the whole year, on three locations and with the four variables**
- **Other sampling schemes provide a quasi similar accuracy**
- **Some sampling schemes are non-optimal**

Results

OED for Dender basin

Non-optimal sampling layouts

Table 1. Non-optimal sampling designs

Sampling interval (h)	Number of samples	Period	Location	Observed variables	Det(FIM)
1	5972	16 Apr.-31 Dec.	Geraardsbergen	DO-NO_3	4,08E+17
1	5340	22 May-15 Nov.	Geraardsbergen	DO-NO_3-BOD	1,19E+19
1	4902	11 May-31 Dec.	Geraardsbergen	DO-NO_3-BOD	5,92E+20

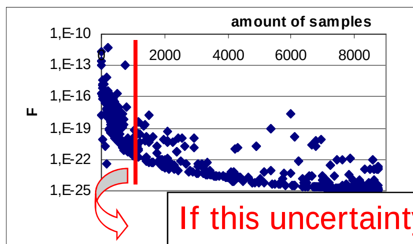
- **Factors that are negative for layout:**
  - **location: upstream**
  - **timing: no measurements in spring**
  - **no NH_4**

Results

OED for Dender basin

Practical considerations

- Final uncertainty on model results is important
  => can be related to cost and practical implications



If this uncertainty is good enough=> 1300 samples instead of 85OO

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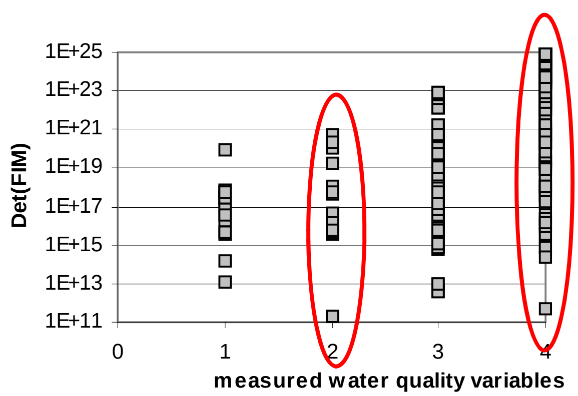
Results

OED for Dender basin

Practical considerations



Replace expensive measurements with cheaper ones?

DO + NO_3 or DO + NO_3 + BOD + NH_4

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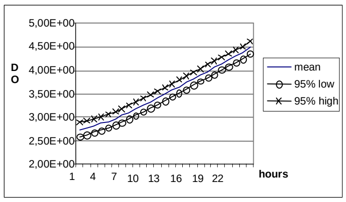
Results

OED for Dender basin

Comparison of three sampling schemes



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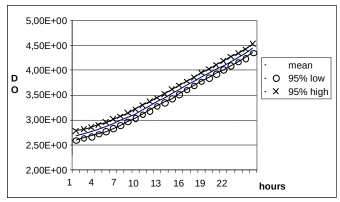

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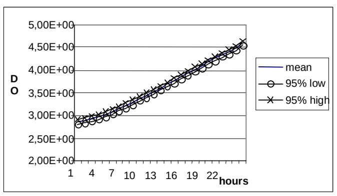

3

- **Average width of the confidence interval around the model results:**
  - **reduction of 45% (2-1)**
  - **reduction of 60% (3-1)**

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Conclusions

- **OED for calibration of water quality models => measurement strategy**
- **Dender: optimal sampling strategy with**
  - **highest number of samples,**
  - **highest sampling frequency,**
  - **maximum number of locations,**
  - **maximum number of variables measured.**
- **Usefulness of the method: evaluation of sub-optimal sampling strategies, in view of limitations, such as costs and practical considerations.**

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